2-Methylnaphthalene

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Model Performance

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N	Model	Data	

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 2.90

Global applicability domain: Inside

Local applicability domain index: 5.95e-01

Confidence level: 7.70e-01

Nearest Neighbors from the Training Set

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Benzene, (2-chloroethyl)-

Measured: 2.95 Predicted: 2.90

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2-Fluorobenzyl chloride

Measured: 2.67 Predicted: 2.91

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Benzene, 1-(chloromethyl)-4-

fluoro-

Measured: 2.73 Predicted: 3.07

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Benzene, 1-(chloromethyl)-3-

fluoro-

Measured: 2.77 Predicted: 3.08

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2-Chlorotoluene Measured: 3.42 Predicted: 2.97